Wei Ku

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Education

1995-2000 **University of Tennessee** Knoxville, TN
Ph.D. Physics -- Thesis "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems"

1994-1995 **Georgia State University** Atlanta, GA
15 credit-hours of course work

1987-1991 **Tamkang University** Tamsui, Taiwan ROC
B.S. Physics

Honors

Lawrence Fellowship in Lawrence Livermore National Lab (2003) (fellowship declined)
Joe Fowler & Jerry Marion Outstanding Graduate Student Award in Department of Physics, University of Tennessee, Knoxville, USA (1998)
Department Head's Award in Department of Physics, TamKang Universy, Tamsui, Taiwan ROC (1988)

Activities

American Physical Society (1999-Present)
Vice president of Chinese Student Association at the University of Tennessee, Knoxville (1997)
UT/ORNL Collaborative Scientist Program (1996-2000)

Skills

All-electron based first-principles many-body theory of condensed matter
Quantum magnetism of highly correlated systems, based on *ab initio* Wannier function analysis
Dynamical charge/magnetic response within time-dependent density functional theory
Quasi-particle excitation spectrum within finite temperature many-body perturbation theory
Quantum Monte Carlo method
Parallel scientific computing (MPI, and OpenMP)
Object-oriented numerical methods
Computer programming: C++, C, FORTRAN, BASIC, and assembly
Platform operation: IBM SP, PC Cluster (with DOS, Windows, or LINUX), Sun Sparc, DEC Alpha, IBM RS6000, and Cray T3E

Relevant Experience

Brookhaven National Laboratory Upton, NY
Assistant Physicist

2003-present First-principles derivation of effective reduced Hamiltonian via numerical CD renormalization group methods

2001-2003 **University of California** Davis, CA
Post-graduate Researcher

Multi-energy-resolution construction of all-electron Wannier functions of highly correlated systems
Microscopic analysis of magnetic structure of spin-Peierls $CuGeO_3$, spin-spiral $CuSiO_3$, and ferromagnetic Li_2CuO_2 chains
Dynamical density response of transition metals and oxides (LDA+U)
Pressure dependence of ferromagnetism of semiconducting EuO, EuS, EuSe, and EuT
Insulating ferromagnetism in half-filled $La_4Ba_2Cu_2O_{10}$
Microscopic origin of complex magnetic structure of $CaCu_3Ti_4O_{12}$
Ab initio construction of 2^{nd}-quantized lattice Hamiltonian using all-electron Wannier functions
Construction of energy-resolved all-electron Wannier function
2D Hubbard model (Quantum Monte Carlo) study of stripes in doped High-Tc superconductors

Collective charge excitations in MgB_2

1997-2000 **University of Tennessee** Knoxville, TN and **Solid State Division, ORNL** Oak Ridge, TN
Graduate Research Assistant

Thesis "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems": first-principles study of electronic excitations in realistic condensed matter within two theoretical frameworks: time-dependent density functional theory (TDDFT), for study of linear density response, and finite-temperature many-body perturbation theory (MBPT) with Kadanoff-Baym conserving (self-consistent) scheme, for study of quasi-particle excitation. Systems studied include simple metals, transition metals and semiconductors.
Quasi-particle excitation spectrum of proto-type semiconductors, Si and Ge
Many-body self-consistency effect on quasi-particle bandwidth of Na
Pure Matsubara time, all-electron, self-consistent *GW* implementation of finite-temperature many-body perturbation theory
d-threshold charge response of Zn and Cd
Absence of Landau damping in Cs
Anomalous plasmon lifetime dispersion of K
All-electron, LAPW implementation of TDDFT linear density response
Proposal, design, construction, and configuration of Linux PC cluster "Hive" in the Solid State Division for parallel computing.

1995-1996 **University of Tennessee** Knoxville, TN
Graduate Teaching Assistant

Undergraduate Lab teaching

1994-1995 **Georgia State University** Atlanta, GA
Graduate Teaching Assistant

Undergraduate Lab teaching

1993-1994 **Tamkang University** Tamsui, Taiwan, ROC
Coordinator of General Physics Lab.

Equipment setup and maintenance for General Physics Lab
Experiment design and improvement
Graduate teaching assistants training and qualifying

Representative Publications

- "Insulating Ferromagnetism in $La_4Ba_4Cu_2O_{10}$: an *Ab Initio* Wannier Function Analysis"
  Wei Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, Phys. Rev. Lett. **89**, 167204 (2002)
- "Band-Gap Problem in Semiconductors Revisited: Effects of Core States and Many-Body Self-Consistency"
  Wei Ku and A. G. Eguiluz, Phys. Rev. Lett. **89**, 126401 (2002)
- "*Ab Initio* Investigation of Collective Charge Excitations in MgB_2"
  Wei Ku, W. E. Pickett, R. T. Scalettar, and A. G. Eguiluz, Phys. Rev. Lett. **88**, 057001 (2002)
- "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Particle Systems"
  Wei Ku, thesis, University of Tennessee, Knoxville (2000)
- "Comment on 'Why is the bandwidth of sodium observed to be narrower in photoemission experiments?' "
  Wei Ku, A. G. Eguiluz, and W. E. Plummer, Phys. Rev. Lett. **85**, 2410 (2000)
- "Plasmon Lifetime in K: A Case Study of Correlated Electrons in Solids Amenable to *Ab Initio* Theory"
  Wei Ku and A. G. Eguiluz, Phys. Rev. Lett. **82**, 2350 (1999)
- "Crucial Role of the Crystal Potential in Magnetism of Edge-Sharing Cu-O Chains and its Interplay with the Bond Angle"
  H. Rosner, Wei Ku, R. T. Scalettar, W. E. Pickett, S.-L. Drechsler, J. Malek, R. Neudert, M. Knupfer, J. Fink, and H. Eschrig, to be submitted to Phys. Rev. Lett.
- "Anomalous Loss Functions of Zn and Cd: Dynamical *d*-Threshold and Coherent Electron-Hole Response"

Wei Ku, and Adolfo G. Eguiluz, to be submitted to Phys. Rev. Lett.

Other Publications

- "Magnetic correlations in manganites probed by resonant inelastic x-ray scattering"
  S. Grenier, J. P. Hill, Wei Ku, V. Kiryukhin, V. Oudovenko, Y.-J. Kim, K. J. Thomas, S.-W. Cheong, Y. Tokura, Y. Tomioka, D. Casa, and T. Gog (preprint)
- "Exchange Coupling in Eu Monochalcogenides from First Principles"
  J. Kunes, Wei Ku, W. E. Pickett (preprint)
- "Giant crystal local-field effects in the dynamical structure factor of rutile TiO2: Theory and experiment"
  I. G. Gurtubay, J. M. Pitarke, W. Ku, A. G. Eguiluz, B. C. Larson, J. Tischler, and P. Zschack (preprint)
- "Effects of the crystal structure in the dynamical electron-density response of hcp transition metals"
  I. G. Gurtubay, Wei Ku, J. M. Pitarke,and A. G. Eguiluz
  Computational Materials Science 30, 104 (2004)
  Selected papers of the Twelfth International Workshop on Computational Materials Science (CMS2002)
- "Self-interaction correction and contact hyperfine field"
  P. Novák, J. Kune, W. E. Pickett, Wei Ku, and F. R. Wagner, Phys. Rev. B **67**, 140403 (2003)
- "PAR-dependent and geometry-dependent mechanisms of spindle positioning"
  M.-F. B. Tsou, Wei Ku, A. Hayashi, and L. S. Rose, J. Cell Bio. **160**, 845 (2003)
- "Microscopic analysis of Insulating Magnetism of $La_4Ba_4Cu_2O_{10}$ and $Nd_4Ba_4Cu_2O_{10}$"
  Wei Ku, H. Rosner, W. E. Pickett, and R. T. Scalettar, J. Solid State Chem. **171**, 329 (2003)
- "MgB_2: Complex Behavior from a Simple Compound"
  H. Rosner, J.M. An, W. Ku, M.D. Johannes, R.T. Scalettar, W.E. Pickett, S.V. Schulga, S.-L. Drechsler, H. Eschrig, W. Weber, and A.G. Eguiluz, Studies of High Temperature Superconductors, Vol. **38**, edited by A. Narlikar (Nova, New York, 2001)
- "Dynamical Response of Correlated Electrons in Solids Probed by Inelastic Scattering Experiments: An *Ab Initio* Theoretical Perspective"
  A. G. Eguiluz, Wei Ku and J. M. Sullivan, J. Phys. Chem. Solids **61**, 383 (2000)
- "*Ab Initio* Studies of Electronic Excitations in Real Solids"
  Adolfo G. Eguiluz and Wei Ku, Electron Correlations and Materials Properties, edited by A. Gonis, N. Kioussis, and M. Ciftan (Kluwer Academic, New York, 1999), p. 329

Invited Presentations

- "Textbook Perturbation Theory at Work in Real Semiconductors:
  What's all the recent arguments on GW calculations about?"
  Department of Physics, Rutgers University (Piscataway, April 2003)
- "First-Principles Methods of Quasi-Particle and Electron-Hole Excitations"
  International Workshop on Computational Materials Physics (Taipei, Taiwan, November 2003)
- "Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation"
  Workshop on Advanced Material Science (Tamsui, Taiwan, November 2003)
- "First-Principles Methods of Quasi-Particle and Electron-Hole Excitations"
  Department of Physics, Tamkang University (Tamsui, Taiwan, November 2003)
- "Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation"
  National Center of Theoretical Sciences (Hsinchu, Taiwan, November 2003)
- "Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation"
  Department of Physics, National Sun Yat-Sen University (Kaohsiung, Taiwan, November 2003)
- "Simple Construction of Energy-Resolved Wannier States with Assigned Local Symmetry"
  CMSN workshop (Knoxville, November 2003)
- "Magnetic Coupling in Insulating Quasi-1D Cu-O Spin Chains: Toward Fully First-Principles Approaches for Strong Correlation"
  Department of Physics, SUNY Stony Brook (Stony Brook, October 2003)
- "Quasi-Particle Excitation in Semiconductors: All-Electron Conserving *GW* scheme"
  ES2003 - Fifteenth Annual Workshop on Recent Developments in Electronic Structure Methods (Minneapolis, May 2003)

- "New Understanding and Surprises from Novel Realistic Many-Body Methods: Quasi-Particle Spectrum of Semiconductors and Insulating Ferromagnetism in Cuprates"
  Lawrence Berkeley National Lab (April, 2003)
- "Wannier Function Study of Insulating Ferromagnetism"
  APS March Meeting (Austin, March 2003)
- "Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories"
  McGill University (Montreal, February 2003)
- "Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories"
  Lawrence Livermore National Laboratory (Livermore, February 2003)
- "Dynamical Electronic Excitations in Real Materials: Perspective of First-Principles Many-Body Theories"
  Brookhaven National Lab (Upton, November 2002)
- "Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$"
  ESCM - Electronic Structure and Computational Magnetism (Washington DC, July 2002)
- "Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$"
  Department of Physics, USC (LA, June 2002)
- "Microscopic Analysis of Non-Metallic Ferromagnetism in $La_4Ba_2Cu_2O_{10}$ Based on *Ab Initio* Wannier Functions"
  Department of Physics, UC Davis (Davis, March 2002)
- "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems"
  Material Research Institute, Lawrence Livermore National Laboratory (Livermore, May 2001)
- "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems"
  Department of Physics, UC Davis (Davis, September 2000)
- "Electronic Excitations in Metals and Semiconductors: *Ab Initio* Studies of Realistic Many-Body systems"
  Solid State Division, Oak Ridge National Laboratory (Oak Ridge, September 2000)
- "Non-uniform Time Axis Technique and All-electron Self-consistent GWA for Si band gap"
  CECAM - Excited states and electronic spectra (Lyon, July 2000)
- "First Principle Study of Electronic Excitation in Condensed Matter: A Bridge Connecting Experiment and Physical Picture"
  Department of Physics, UT Knoxville (Knoxville, April 2000)
- "Collective Modes in Simple Metals: Plasmon, Zone Boundary Collective State, and Core Dipole Collective Mode"
  Department of Physics, UT Knoxville (Knoxville, September 1998)

Presentations/ Conferences

- CFN Users' Meeting, BNL (Upton, May 2004)
- "Theoretical Study of Magnetic, Orbital and Lattice Structure of MnF3: Is Jahn-Teller Distortion Necessary for Orbital Ordering?"
  NSLS annual users' meeting, BNL (Upton, May 2004) (poster)
- "Origin of Magnetic Coupling in Quasi-1D Edge-Sharing Cu-O Chains: Role of the Crystal Potential"
  Department of Physics, BNL (Upton, April 2004)
- "Trend of Tc_max in High-Tc materials? An analysis of t and t' with Wannier functions."
  Department of Physics, BNL (Upton, April 2004)
- "Trend of Tc_max in High-Tc materials? An analysis of t and t' with Wannier functions."
  CMSN workshop (Montreal, March 2004)
- "Trend of Tc_max in High-Tc materials? An analysis of t and t' with Wannier functions."
  APS March Meeting (Montreal, March 2004)
- "Theoretical Perspectives on IXS"
  Workshop for NSLS-II: The Future National Synchrotron Light Source (BNL, March 2004)
- "Density Functional Theory, its Extension, and Applications on Solids"

lecture in Department of Physics, SUNY Stony Brook (Stony Brook, October 2003)

- International Workshop on Field Theory Methods in Correlated Nanoscale Systems (BNL, August 2003)
- Strongly Correlated Electrons: NSLS II and the Future (BNL, August 2003)
- "Origin of Magnetic Coupling in Quasi-1D Edge-Sharing Cu-O Chains: Role of the Crystal Potential"
  "Dynamical Charge Response of NiO"
  "Charge-Transfer Gap of CaB6: Large Effect of Many-Body Self-Consistency"
  APS March Meeting (Austin, March 2003)
- "From weak correlation to strong correlation: *ab initio* many body theory of the next generation"
  CMSN workshop (Davis, January 2003)
- "All-Electron, Conserving Investigation of the Band Gap of Si and Ge: Effects of Core States and Many-Body Self-Consistency"
  KITP program "Realistic Theories of Correlated Electron Materials" (Santa Barbara, September 2002)
- "Microscopic Analysis of Insulating Magnetism of $La_4Ba_2Cu_2O_{10}$ and $Nd_4Ba_2Cu_2O_{10}$"
  RERC - Rare Earth Research Conference (Davis, July 2002) (poster)
- Conference on Current Issues in the Optical Response of Solid Materials (Irvine, June 2002)
- "Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$"
  "All-Electron, Conserving *GW* calculation of the Quasi-Particle Band Gap in Si and Ge: Effects of the Deep Core States and Many-Body Self-consistency"
  ES2002 - Annual Workshop on Recent Developments in Electronic Structure Methods (Berkeley, June 2002) (poster)
- "Microscopic Analysis of Non-Metallic Ferromagnetism in $La_4Ba_2Cu_2O_{10}$ Based on *Ab Initio* Wannier Functions"
  APS March Meeting California session (Davis, March 2002)
- "Microscopic Analysis of Non-Metallic Ferromagnetism in $La_4Ba_2Cu_2O_{10}$ Based on *Ab Initio* Wannier Functions"
  "Dynamical Charge Fluctuations in MgB_2 and the Superconductivity Mechanism"
  "Inelastic X-Ray Scattering Investigations of Electron Dynamics in Copper"
  "Dynamical Density Response of Metals with Narrow Bands: The Cases of Cr, Ga, and In"
  APS March Meeting (Indianapolis, March 2002)
- "*Ab Initio* Investigation of Collective Charge Excitations in MgB_2"
  CMSN - Workshop on Excited State Properties and Response Functions for Materials, LBNL (Berkeley, October, 2001)
- ALS / MES / SRRTNet Workshop on Molecular Environmental Science and Theory, Computation and Synchrotron Experiments, LBNL (Berkeley, October 2001)
- Conference on Strongly Correlated Electron Systems (SCES2001) (Ann Arbor, July 2001)
- "All-Electron, Conserving Investigation of the Band Gap of Si and Ge within the *GW* Approximation"
  "Electron-Hole Excitations in Post-Transition Metals Zn and Cd: a Novel Theoretical Perspective"
  APS March meeting (Seattle, March 2001)
- "Probing the Electronic Correlations in Condensed Matter with Inelastic Scattering of X-rays"
  Division of Material Sciences & Engineering Condensed Matter Physics and Material Chemistry Program Review, ONRL (Oak Ridge, September 2000) (poster)
- Workshop on Soft X-Ray Science in the Next Millennium: The Future of Photon-In/Photon-Out Experiments (Pikeville, March 2000)
- "Plasmon Lifetime in K: A Case Study of Correlated Electrons in Solids Amenable to *Ab Initio* Theory"
  "Electronic Excitations in Transition Metals of the 3d and 4d Rows with Shallow Core States"
  APS March meeting (Atlanta, March 1999)

References

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